



wwPDB X-ray Structure Validation Summary Report i

Feb 26, 2014 – 02:41 PM GMT

PDB ID : 3SM5
Title : Influenza hemagglutinin in complex with a neutralizing antibody
Authors : Whittle, J.R.R.; Harrison, S.C.
Deposited on : 2011-06-27
Resolution : 3.19 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

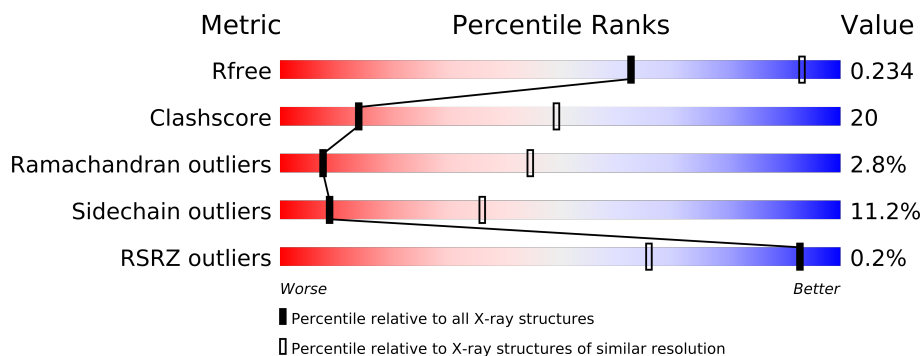
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.19 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	327	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	C	327	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	E	327	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
2	B	182	<div><div></div><div><div></div><div></div><div></div><div></div></div><div></div></div>
2	D	182	<div><div></div><div><div></div><div></div><div></div><div></div></div><div></div></div>
2	F	182	<div><div></div><div><div></div><div></div><div></div><div></div></div><div></div></div>
3	H	227	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
3	I	227	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
3	J	227	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
4	L	211	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
4	M	211	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
4	N	211	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>

The following table lists non-polymeric compounds that are outliers for geometric or electron-

density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
7	NAG	A	341	-	X
7	NAG	C	351	-	X
7	NAG	C	371	-	X
7	NAG	E	341	-	X
7	NAG	E	371	-	X
9	SO4	A	337	-	X
9	SO4	C	337	-	X
9	SO4	C	339	-	X
9	SO4	C	340	-	X
9	SO4	E	335	-	X
9	SO4	E	339	-	X
9	SO4	E	340	-	X
9	SO4	E	342	-	X
9	SO4	E	345	-	X
9	SO4	E	346	-	X
9	SO4	I	229	-	X
9	SO4	L	213	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 22009 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2535	1597	441	486	11			
1	C	323	Total	C	N	O	S	0	0	0
			2535	1597	441	486	11			
1	E	323	Total	C	N	O	S	0	0	0
			2535	1597	441	486	11			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	GLU	-	EXPRESSION TAG	UNP A7UPX0
C	4	GLU	-	EXPRESSION TAG	UNP A7UPX0
E	4	GLU	-	EXPRESSION TAG	UNP A7UPX0

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	173	Total	C	N	O	S	0	0	0
			1391	871	238	275	7			
2	D	173	Total	C	N	O	S	0	0	0
			1391	871	238	275	7			
2	F	173	Total	C	N	O	S	0	0	0
			1391	871	238	275	7			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	677	ARG	-	EXPRESSION TAG	UNP C5H943
B	678	SER	-	EXPRESSION TAG	UNP C5H943
B	679	LEU	-	EXPRESSION TAG	UNP C5H943
B	680	VAL	-	EXPRESSION TAG	UNP C5H943
B	681	PRO	-	EXPRESSION TAG	UNP C5H943

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Chain	Residue	Modelled	Actual	Comment	Reference
B	682	ARG	-	EXPRESSION TAG	UNP C5H943
D	677	ARG	-	EXPRESSION TAG	UNP C5H943
D	678	SER	-	EXPRESSION TAG	UNP C5H943
D	679	LEU	-	EXPRESSION TAG	UNP C5H943
D	680	VAL	-	EXPRESSION TAG	UNP C5H943
D	681	PRO	-	EXPRESSION TAG	UNP C5H943
D	682	ARG	-	EXPRESSION TAG	UNP C5H943
F	677	ARG	-	EXPRESSION TAG	UNP C5H943
F	678	SER	-	EXPRESSION TAG	UNP C5H943
F	679	LEU	-	EXPRESSION TAG	UNP C5H943
F	680	VAL	-	EXPRESSION TAG	UNP C5H943
F	681	PRO	-	EXPRESSION TAG	UNP C5H943
F	682	ARG	-	EXPRESSION TAG	UNP C5H943

- Molecule 3 is a protein called CH65, heavy chain, Fab fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	221	Total	C	N	O	S	0	0	0
			1673	1059	278	328	8			
3	I	221	Total	C	N	O	S	0	0	0
			1673	1059	278	328	8			
3	J	221	Total	C	N	O	S	0	0	0
			1673	1059	278	328	8			

- Molecule 4 is a protein called CH65, light chain, Fab fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	210	Total	C	N	O	S	0	0	0
			1565	973	269	318	5			
4	M	210	Total	C	N	O	S	0	0	0
			1565	973	269	318	5			
4	N	210	Total	C	N	O	S	0	0	0
			1565	973	269	318	5			

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	2	Total	C	N	O	0	0
			28	16	2	10		
5	A	2	Total	C	N	O	0	0
			28	16	2	10		

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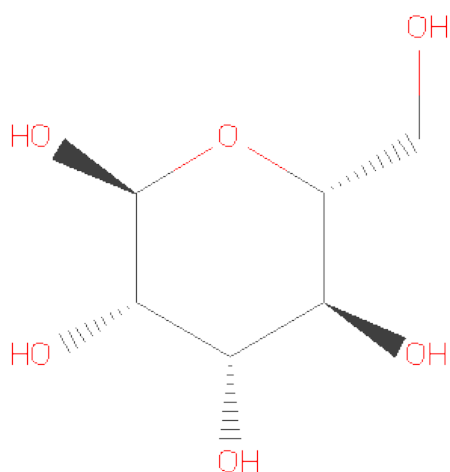
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	2	Total	C	N	O	0	0
			28	16	2	10		
5	C	2	Total	C	N	O	0	0
			28	16	2	10		
5	E	2	Total	C	N	O	0	0
			28	16	2	10		

There are 5 discrepancies between the modelled and reference sequences:

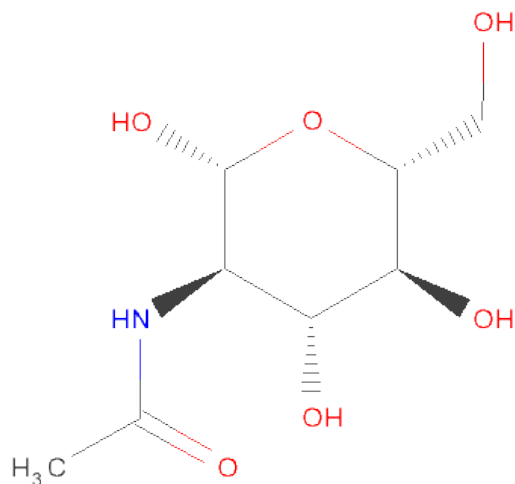
Chain	Residue	Modelled	Actual	Comment	Reference
A	4	GLU	-	EXPRESSION TAG	UNP A7UPX0
A	4	GLU	-	EXPRESSION TAG	UNP A7UPX0
C	4	GLU	-	EXPRESSION TAG	UNP A7UPX0
C	4	GLU	-	EXPRESSION TAG	UNP A7UPX0
E	4	GLU	-	EXPRESSION TAG	UNP A7UPX0

- Molecule 6 is SUGAR (ALPHA-D-MANNOSE) (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 7 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	C	1	Total	C	N	O	0	0
			14	8	1	5		
7	E	1	Total	C	N	O	0	0
			14	8	1	5		
7	E	1	Total	C	N	O	0	0
			14	8	1	5		
7	E	1	Total	C	N	O	0	0
			14	8	1	5		

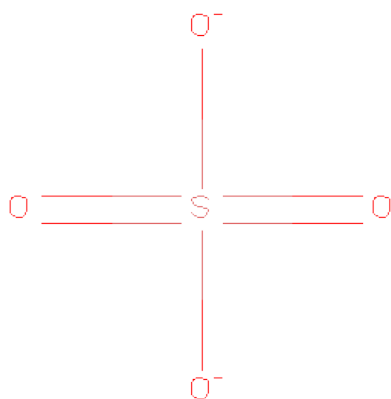
- Molecule 8 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	E	3	Total	C	N	O	0	0
			39	22	2	15		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	4	GLU	-	EXPRESSION TAG	UNP A7UPX0

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	H	1	Total	O	S	0	0
			5	4	1		
9	J	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		
9	E	1	Total	O	S	0	0
			5	4	1		
9	A	1	Total	O	S	0	0
			5	4	1		
9	E	1	Total	O	S	0	0
			5	4	1		
9	I	1	Total	O	S	0	0
			5	4	1		
9	H	1	Total	O	S	0	0
			5	4	1		
9	I	1	Total	O	S	0	0
			5	4	1		
9	A	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		
9	E	1	Total	O	S	0	0
			5	4	1		
9	N	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	J	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		
9	E	1	Total	O	S	0	0
			5	4	1		
9	E	1	Total	O	S	0	0
			5	4	1		
9	A	1	Total	O	S	0	0
			5	4	1		
9	H	1	Total	O	S	0	0
			5	4	1		
9	N	1	Total	O	S	0	0
			5	4	1		
9	L	1	Total	O	S	0	0
			5	4	1		
9	E	1	Total	O	S	0	0
			5	4	1		
9	A	1	Total	O	S	0	0
			5	4	1		
9	M	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		
9	A	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		
9	I	1	Total	O	S	0	0
			5	4	1		
9	E	1	Total	O	S	0	0
			5	4	1		
9	E	1	Total	O	S	0	0
			5	4	1		
9	E	1	Total	O	S	0	0
			5	4	1		
9	L	1	Total	O	S	0	0
			5	4	1		
9	N	1	Total	O	S	0	0
			5	4	1		

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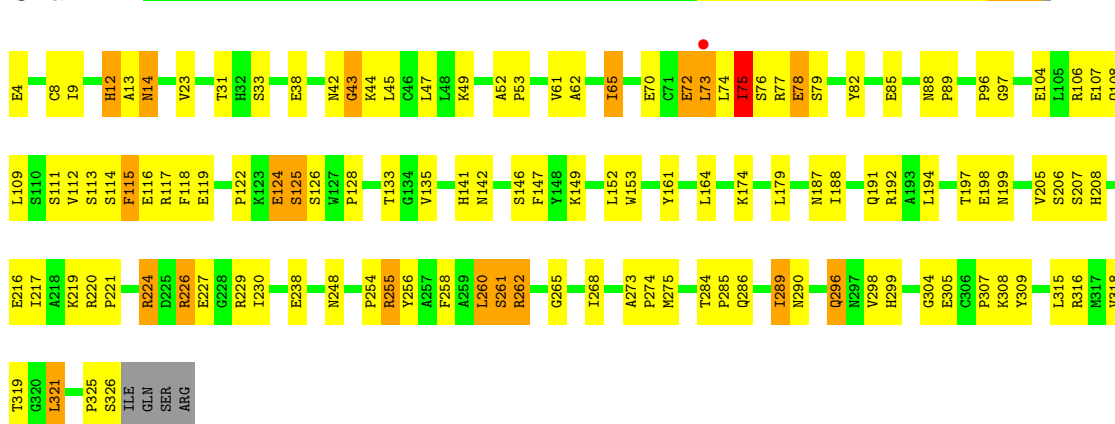
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		
9	E	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		
9	E	1	Total	O	S	0	0
			5	4	1		
9	E	1	Total	O	S	0	0
			5	4	1		
9	I	1	Total	O	S	0	0
			5	4	1		
9	I	1	Total	O	S	0	0
			5	4	1		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

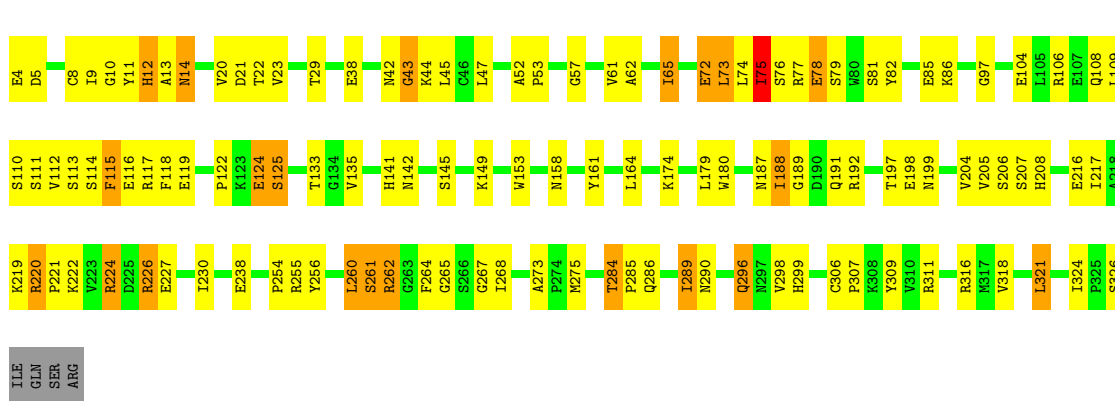
• Molecule 1: Hemagglutinin

Chain A:



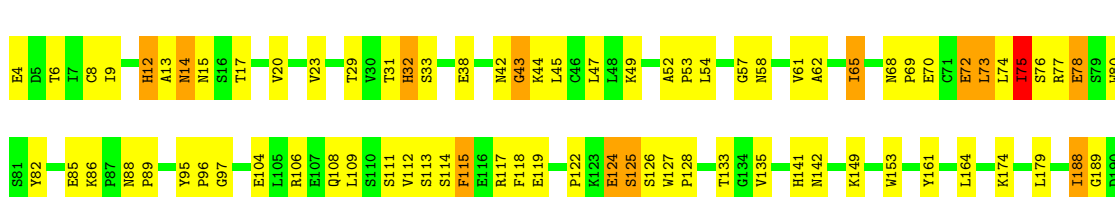
• Molecule 1: Hemagglutinin

Chain C:



• Molecule 1: Hemagglutinin

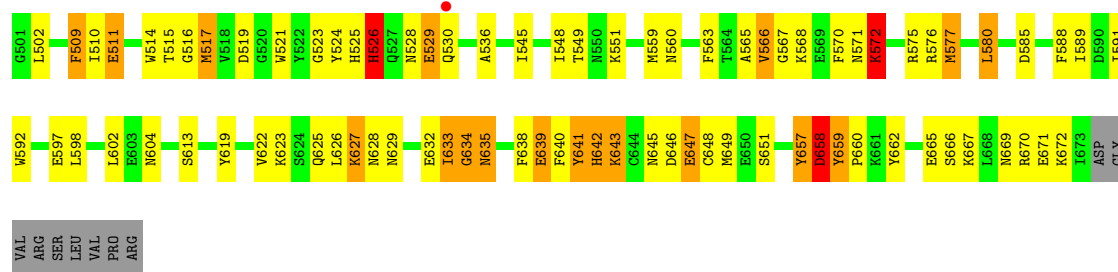
Chain E:





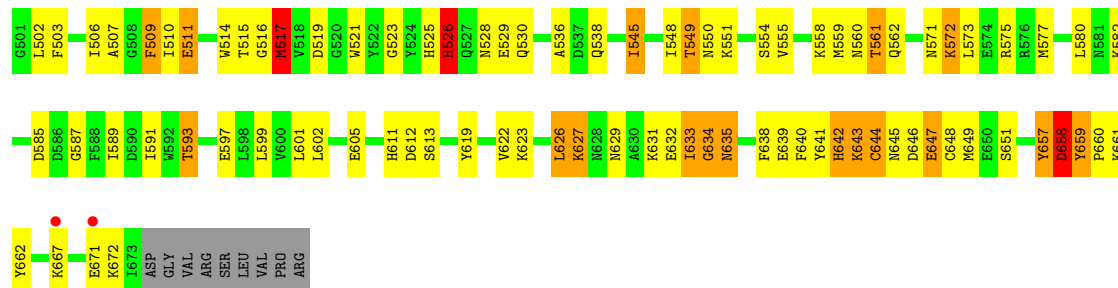
• Molecule 2: Hemagglutinin

Chain B:



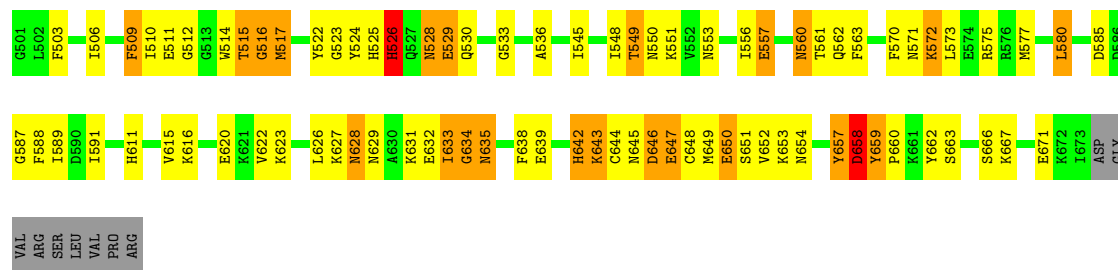
• Molecule 2: Hemagglutinin

Chain D:



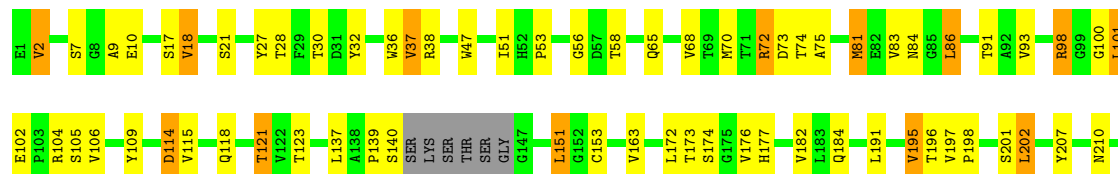
• Molecule 2: Hemagglutinin

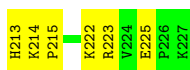
Chain F:



• Molecule 3: CH65, heavy chain, Fab fragment

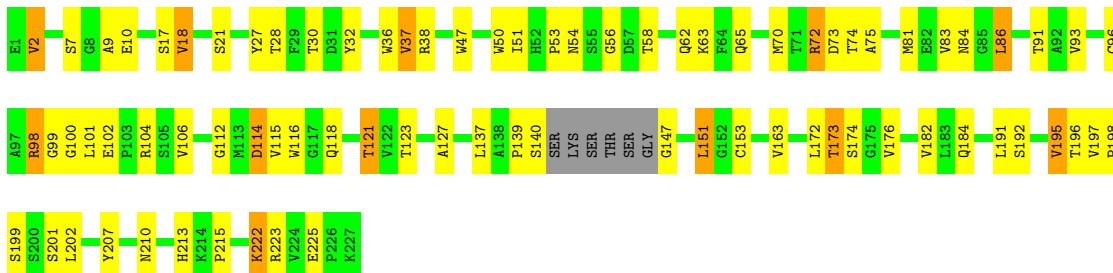
Chain H:





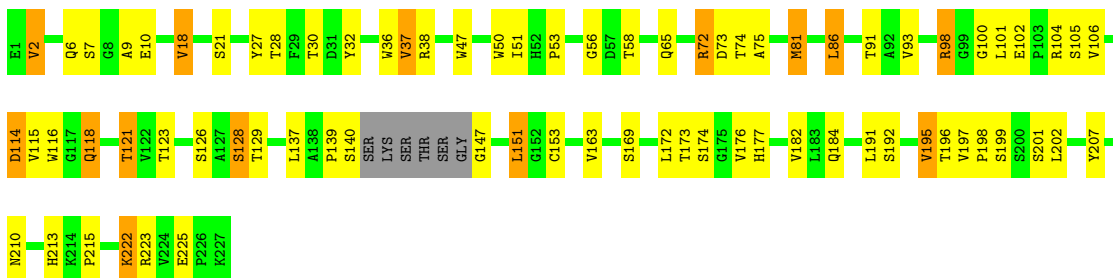
- Molecule 3: CH65, heavy chain, Fab fragment

Chain I:



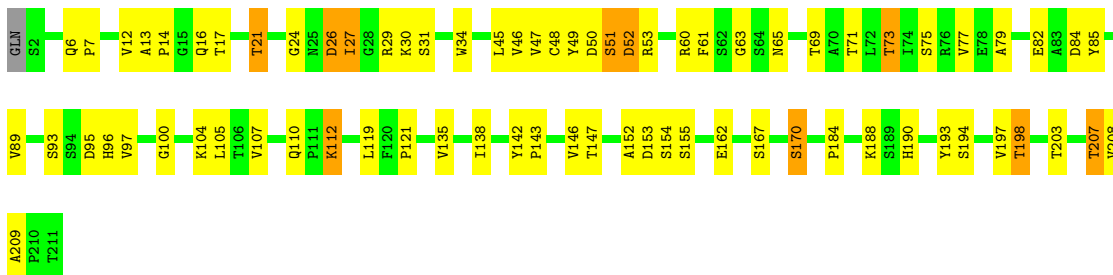
- Molecule 3: CH65, heavy chain, Fab fragment

Chain J:



- Molecule 4: CH65, light chain, Fab fragment

Chain L:



- Molecule 4: CH65, light chain, Fab fragment

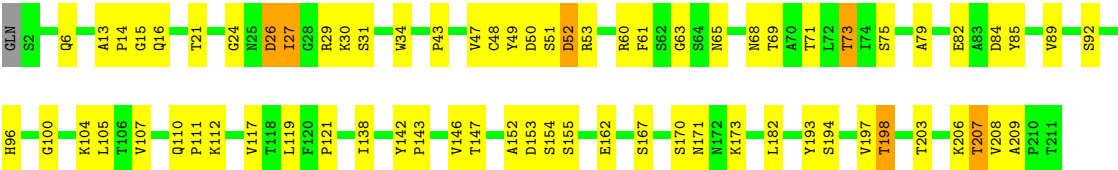
Chain M:



- Molecule 4: CH65, light chain, Fab fragment

Chain N:





4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	154.98Å 191.84Å 332.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.09 – 3.19 30.09 – 3.19	Depositor EDS
% Data completeness (in resolution range)	98.0 (30.09-3.19) 92.4 (30.09-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 3.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.211 , 0.249 0.198 , 0.234	Depositor DCC
R_{free} test set	1869 reflections (2.47%)	DCC
Wilson B-factor (Å ²)	80.3	Xtriage
Anisotropy	0.571	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 39.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 80373 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	22009	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, BMA, NAG, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.46	0/2601	0.62	0/3540
1	C	0.47	0/2601	0.62	0/3540
1	E	0.47	0/2601	0.61	0/3540
2	B	0.45	0/1418	0.65	0/1905
2	D	0.47	0/1418	0.63	0/1905
2	F	0.51	0/1418	0.67	0/1905
3	H	0.51	0/1718	0.65	0/2347
3	I	0.51	0/1718	0.65	0/2347
3	J	0.54	0/1718	0.64	0/2347
4	L	0.45	0/1603	0.60	0/2192
4	M	0.45	0/1603	0.60	0/2192
4	N	0.46	0/1603	0.61	0/2192
All	All	0.48	0/22020	0.63	0/29952

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	E	1	0

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	E	351	NAG	C1

There are no planarity outliers.

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2535	0	2441	112	0
1	C	2535	0	2438	119	0
1	E	2535	0	2440	111	0
2	B	1391	0	1316	93	0
2	D	1391	0	1316	112	0
2	F	1391	0	1316	109	0
3	H	1673	0	1606	48	0
3	I	1673	0	1606	50	0
3	J	1673	0	1606	42	0
4	L	1565	0	1513	60	0
4	M	1565	0	1513	47	0
4	N	1565	0	1513	49	0
5	A	56	0	50	3	0
5	C	56	0	50	2	0
5	E	28	0	25	3	0
6	A	11	0	10	0	0
7	A	28	0	26	2	0
7	C	42	0	39	0	0
7	E	42	0	39	4	0
8	E	39	0	34	7	0
9	A	30	0	0	1	0
9	C	45	0	0	6	0
9	E	60	0	0	4	0
9	H	15	0	0	1	0
9	I	25	0	0	1	0
9	J	10	0	0	0	0
9	L	10	0	0	1	0
9	M	5	0	0	0	0
9	N	15	0	0	1	0
All	All	22009	0	20897	851	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 20.

The worst 5 of 851 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:519:ASP:HB2	2:D:536:ALA:HB3	1.45	0.97
1:E:77:ARG:NH1	9:E:344:SO4:O4	1.99	0.96
3:H:18:VAL:HG22	3:H:86:LEU:HD21	1.47	0.95
1:E:70:GLU:HG3	8:E:331:NAG:HN2	1.31	0.95
2:D:642:HIS:O	2:D:642:HIS:ND1	2.01	0.94

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	321/327 (98%)	285 (89%)	29 (9%)	7 (2%)	10	53
1	C	321/327 (98%)	286 (89%)	27 (8%)	8 (2%)	9	49
1	E	321/327 (98%)	284 (88%)	30 (9%)	7 (2%)	10	53
2	B	171/182 (94%)	129 (75%)	28 (16%)	14 (8%)	1	10
2	D	171/182 (94%)	133 (78%)	26 (15%)	12 (7%)	2	13
2	F	171/182 (94%)	135 (79%)	23 (14%)	13 (8%)	2	12
3	H	217/227 (96%)	197 (91%)	18 (8%)	2 (1%)	25	76
3	I	217/227 (96%)	198 (91%)	16 (7%)	3 (1%)	16	66
3	J	217/227 (96%)	196 (90%)	19 (9%)	2 (1%)	25	76
4	L	208/211 (99%)	186 (89%)	19 (9%)	3 (1%)	16	66
4	M	208/211 (99%)	189 (91%)	16 (8%)	3 (1%)	16	66
4	N	208/211 (99%)	189 (91%)	16 (8%)	3 (1%)	16	66
All	All	2751/2841 (97%)	2407 (88%)	267 (10%)	77 (3%)	8	44

5 of 77 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	ILE
2	B	643	LYS
1	C	125	SER

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Mol	Chain	Res	Type
2	D	526	HIS
2	D	627	LYS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	283/287 (99%)	257 (91%)	26 (9%)	13	47
1	C	283/287 (99%)	254 (90%)	29 (10%)	11	40
1	E	283/287 (99%)	254 (90%)	29 (10%)	11	40
2	B	148/157 (94%)	130 (88%)	18 (12%)	7	31
2	D	148/157 (94%)	125 (84%)	23 (16%)	4	17
2	F	148/157 (94%)	130 (88%)	18 (12%)	7	31
3	H	184/190 (97%)	158 (86%)	26 (14%)	5	23
3	I	184/190 (97%)	159 (86%)	25 (14%)	5	25
3	J	184/190 (97%)	153 (83%)	31 (17%)	3	14
4	L	177/178 (99%)	162 (92%)	15 (8%)	15	53
4	M	177/178 (99%)	164 (93%)	13 (7%)	20	62
4	N	177/178 (99%)	163 (92%)	14 (8%)	18	58
All	All	2376/2436 (98%)	2109 (89%)	267 (11%)	9	36

5 of 267 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	284	THR
3	H	72	ARG
4	M	73	THR
1	E	326	SER
2	F	573	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	286	GLN
2	D	530	GLN
3	I	54	ASN
2	B	669	ASN
1	C	187	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

13 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	A	331	1,5	12,14,15	0.74	1 (8%)	15,19,21	1.15	1 (6%)
5	NAG	A	332	5	12,14,15	0.59	0	15,19,21	1.86	3 (20%)
5	NAG	A	371	1,5	12,14,15	0.67	1 (8%)	15,19,21	1.21	1 (6%)
5	NAG	A	372	5	12,14,15	0.63	0	15,19,21	1.22	1 (6%)
5	NAG	C	331	1,5	12,14,15	0.51	0	15,19,21	1.91	3 (20%)
5	NAG	C	332	5	12,14,15	0.70	0	15,19,21	1.31	3 (20%)
5	NAG	C	341	1,5	12,14,15	0.58	0	15,19,21	1.77	2 (13%)
5	NAG	C	342	5	12,14,15	0.63	0	15,19,21	1.34	1 (6%)
8	NAG	E	331	1,8	12,14,15	0.82	1 (8%)	15,19,21	0.90	0
8	NAG	E	332	8	12,14,15	0.82	0	15,19,21	1.34	4 (26%)
8	BMA	E	333	8	10,11,12	0.62	0	11,15,17	1.55	1 (9%)
5	NAG	E	351	1,5	12,14,15	0.81	1 (8%)	15,19,21	1.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	E	352	5	12,14,15	0.67	0	15,19,21	1.61	2 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	331	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	332	5	-	2/6/23/26	0/1/1/1
5	NAG	A	371	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	372	5	-	2/6/23/26	0/1/1/1
5	NAG	C	331	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	332	5	-	0/6/23/26	0/1/1/1
5	NAG	C	341	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	342	5	-	0/6/23/26	0/1/1/1
8	NAG	E	331	1,8	-	0/6/23/26	0/1/1/1
8	NAG	E	332	8	-	0/6/23/26	0/1/1/1
8	BMA	E	333	8	-	0/2/19/22	0/1/1/1
5	NAG	E	351	1,5	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	E	352	5	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	E	331	NAG	O5-C5	-2.36	1.41	1.45
5	E	351	NAG	O5-C5	-2.34	1.41	1.45
5	A	331	NAG	O5-C5	-2.11	1.41	1.45
5	A	371	NAG	O5-C5	-2.04	1.41	1.45

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	331	NAG	O5-C5-C4	5.76	117.96	110.65
5	A	332	NAG	O5-C5-C6	5.62	112.88	106.98
5	C	341	NAG	O5-C5-C6	5.16	112.40	106.98
5	E	352	NAG	C2-N2-C7	4.42	130.51	123.09
8	E	333	BMA	O5-C5-C6	4.25	111.44	106.98

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	E	351	NAG	C1

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	332	NAG	C1-C2-N2-C7
5	A	372	NAG	C3-C2-N2-C7
5	A	372	NAG	O7-C7-N2-C2
5	A	332	NAG	O7-C7-N2-C2

There are no ring outliers.

5.6 Ligand geometry ⓘ

52 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	MAN	A	333	-	10,11,12	0.72	0	11,15,17	1.14	1 (9%)
9	SO4	A	334	-	4,4,4	0.09	0	6,6,6	0.30	0
9	SO4	A	335	-	4,4,4	0.09	0	6,6,6	0.36	0
9	SO4	A	336	-	4,4,4	0.15	0	6,6,6	0.19	0
9	SO4	A	337	-	4,4,4	0.13	0	6,6,6	0.22	0
9	SO4	A	338	-	4,4,4	0.09	0	6,6,6	0.11	0
9	SO4	A	339	-	4,4,4	0.13	0	6,6,6	0.18	0
7	NAG	A	341	1	12,14,15	0.50	0	15,19,21	1.48	2 (13%)
7	NAG	A	361	1	12,14,15	0.53	0	15,19,21	1.92	2 (13%)
9	SO4	C	333	-	4,4,4	0.11	0	6,6,6	0.39	0
9	SO4	C	334	-	4,4,4	0.38	0	6,6,6	0.73	0
9	SO4	C	335	-	4,4,4	0.13	0	6,6,6	0.22	0
9	SO4	C	336	-	4,4,4	0.10	0	6,6,6	0.27	0
9	SO4	C	337	-	4,4,4	0.19	0	6,6,6	0.41	0
9	SO4	C	338	-	4,4,4	0.15	0	6,6,6	0.31	0
9	SO4	C	339	-	4,4,4	0.18	0	6,6,6	0.07	0
9	SO4	C	340	-	4,4,4	0.42	0	6,6,6	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	SO4	C	343	-	4,4,4	0.54	0	6,6,6	0.33	0
7	NAG	C	351	1	12,14,15	0.68	0	15,19,21	0.98	2 (13%)
7	NAG	C	361	1	12,14,15	0.65	0	15,19,21	1.45	1 (6%)
7	NAG	C	371	1	12,14,15	0.60	0	15,19,21	1.40	2 (13%)
9	SO4	E	334	-	4,4,4	0.14	0	6,6,6	0.32	0
9	SO4	E	335	-	4,4,4	0.14	0	6,6,6	0.19	0
9	SO4	E	336	-	4,4,4	0.22	0	6,6,6	0.23	0
9	SO4	E	337	-	4,4,4	0.23	0	6,6,6	0.25	0
9	SO4	E	338	-	4,4,4	0.10	0	6,6,6	0.18	0
9	SO4	E	339	-	4,4,4	0.17	0	6,6,6	0.17	0
9	SO4	E	340	-	4,4,4	0.16	0	6,6,6	0.15	0
7	NAG	E	341	1	12,14,15	0.46	0	15,19,21	1.72	4 (26%)
9	SO4	E	342	-	4,4,4	0.09	0	6,6,6	0.23	0
9	SO4	E	343	-	4,4,4	0.12	0	6,6,6	0.12	0
9	SO4	E	344	-	4,4,4	0.28	0	6,6,6	0.28	0
9	SO4	E	345	-	4,4,4	0.43	0	6,6,6	0.11	0
9	SO4	E	346	-	4,4,4	0.57	0	6,6,6	0.64	0
7	NAG	E	361	1	12,14,15	0.63	0	15,19,21	1.16	1 (6%)
7	NAG	E	371	1	12,14,15	0.56	0	15,19,21	1.54	1 (6%)
9	SO4	H	228	-	4,4,4	0.26	0	6,6,6	0.37	0
9	SO4	H	229	-	4,4,4	0.16	0	6,6,6	0.33	0
9	SO4	H	230	-	4,4,4	0.19	0	6,6,6	0.26	0
9	SO4	I	228	-	4,4,4	0.11	0	6,6,6	0.22	0
9	SO4	I	229	-	4,4,4	0.10	0	6,6,6	0.26	0
9	SO4	I	230	-	4,4,4	0.17	0	6,6,6	0.17	0
9	SO4	I	231	-	4,4,4	0.17	0	6,6,6	0.35	0
9	SO4	I	232	-	4,4,4	0.32	0	6,6,6	0.52	0
9	SO4	J	228	-	4,4,4	0.32	0	6,6,6	0.68	0
9	SO4	J	229	-	4,4,4	0.26	0	6,6,6	0.53	0
9	SO4	L	212	-	4,4,4	0.11	0	6,6,6	0.16	0
9	SO4	L	213	-	4,4,4	0.11	0	6,6,6	0.23	0
9	SO4	M	212	-	4,4,4	0.12	0	6,6,6	0.25	0
9	SO4	N	212	-	4,4,4	0.19	0	6,6,6	0.36	0
9	SO4	N	213	-	4,4,4	0.10	0	6,6,6	0.46	0
9	SO4	N	214	-	4,4,4	0.19	0	6,6,6	0.33	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MAN	A	333	-	-	0/2/19/22	0/1/1/1
9	SO4	A	334	-	-	0/0/0/0	0/0/0/0
9	SO4	A	335	-	-	0/0/0/0	0/0/0/0
9	SO4	A	336	-	-	0/0/0/0	0/0/0/0
9	SO4	A	337	-	-	0/0/0/0	0/0/0/0
9	SO4	A	338	-	-	0/0/0/0	0/0/0/0
9	SO4	A	339	-	-	0/0/0/0	0/0/0/0
7	NAG	A	341	1	-	0/6/23/26	0/1/1/1
7	NAG	A	361	1	-	2/6/23/26	0/1/1/1
9	SO4	C	333	-	-	0/0/0/0	0/0/0/0
9	SO4	C	334	-	-	0/0/0/0	0/0/0/0
9	SO4	C	335	-	-	0/0/0/0	0/0/0/0
9	SO4	C	336	-	-	0/0/0/0	0/0/0/0
9	SO4	C	337	-	-	0/0/0/0	0/0/0/0
9	SO4	C	338	-	-	0/0/0/0	0/0/0/0
9	SO4	C	339	-	-	0/0/0/0	0/0/0/0
9	SO4	C	340	-	-	0/0/0/0	0/0/0/0
9	SO4	C	343	-	-	0/0/0/0	0/0/0/0
7	NAG	C	351	1	-	0/6/23/26	0/1/1/1
7	NAG	C	361	1	-	0/6/23/26	0/1/1/1
7	NAG	C	371	1	-	0/6/23/26	0/1/1/1
9	SO4	E	334	-	-	0/0/0/0	0/0/0/0
9	SO4	E	335	-	-	0/0/0/0	0/0/0/0
9	SO4	E	336	-	-	0/0/0/0	0/0/0/0
9	SO4	E	337	-	-	0/0/0/0	0/0/0/0
9	SO4	E	338	-	-	0/0/0/0	0/0/0/0
9	SO4	E	339	-	-	0/0/0/0	0/0/0/0
9	SO4	E	340	-	-	0/0/0/0	0/0/0/0
7	NAG	E	341	1	-	0/6/23/26	0/1/1/1
9	SO4	E	342	-	-	0/0/0/0	0/0/0/0
9	SO4	E	343	-	-	0/0/0/0	0/0/0/0
9	SO4	E	344	-	-	0/0/0/0	0/0/0/0
9	SO4	E	345	-	-	0/0/0/0	0/0/0/0
9	SO4	E	346	-	-	0/0/0/0	0/0/0/0
7	NAG	E	361	1	-	0/6/23/26	0/1/1/1
7	NAG	E	371	1	-	0/6/23/26	0/1/1/1
9	SO4	H	228	-	-	0/0/0/0	0/0/0/0
9	SO4	H	229	-	-	0/0/0/0	0/0/0/0
9	SO4	H	230	-	-	0/0/0/0	0/0/0/0
9	SO4	I	228	-	-	0/0/0/0	0/0/0/0
9	SO4	I	229	-	-	0/0/0/0	0/0/0/0
9	SO4	I	230	-	-	0/0/0/0	0/0/0/0
9	SO4	I	231	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	SO4	I	232	-	-	0/0/0/0	0/0/0/0
9	SO4	J	228	-	-	0/0/0/0	0/0/0/0
9	SO4	J	229	-	-	0/0/0/0	0/0/0/0
9	SO4	L	212	-	-	0/0/0/0	0/0/0/0
9	SO4	L	213	-	-	0/0/0/0	0/0/0/0
9	SO4	M	212	-	-	0/0/0/0	0/0/0/0
9	SO4	N	212	-	-	0/0/0/0	0/0/0/0
9	SO4	N	213	-	-	0/0/0/0	0/0/0/0
9	SO4	N	214	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	361	NAG	O5-C5-C6	6.55	113.85	106.98
7	E	371	NAG	O5-C5-C6	4.93	112.16	106.98
7	C	361	NAG	O5-C5-C6	4.62	111.83	106.98
7	A	341	NAG	O5-C5-C4	3.63	115.26	110.65
7	E	361	NAG	O5-C5-C6	3.49	110.64	106.98

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	361	NAG	O7-C7-N2-C2
7	A	361	NAG	C8-C7-N2-C2

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	323/327 (98%)	-0.17	1 (0%) 91 58	70, 90, 118, 146	0
1	C	323/327 (98%)	-0.15	0 100 100	67, 88, 115, 145	0
1	E	323/327 (98%)	-0.17	0 100 100	66, 87, 116, 144	0
2	B	173/182 (95%)	-0.12	1 (0%) 86 41	63, 102, 143, 158	0
2	D	173/182 (95%)	-0.08	2 (1%) 75 26	55, 101, 150, 170	0
2	F	173/182 (95%)	-0.13	0 100 100	60, 92, 146, 168	0
3	H	221/227 (97%)	-0.21	0 100 100	61, 79, 111, 133	0
3	I	221/227 (97%)	-0.22	0 100 100	61, 78, 114, 134	0
3	J	221/227 (97%)	-0.20	0 100 100	58, 77, 112, 134	0
4	L	210/211 (99%)	-0.15	0 100 100	70, 92, 113, 136	0
4	M	210/211 (99%)	-0.18	0 100 100	68, 90, 112, 134	0
4	N	210/211 (99%)	-0.21	0 100 100	68, 88, 110, 133	0
All	All	2781/2841 (97%)	-0.17	4 (0%) 93 74	55, 87, 127, 170	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	73	LEU	2.3
2	D	667	LYS	2.2
2	B	530	GLN	2.1
2	D	671	GLU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	NAG	C	341	14/15	0.40	8.88	120,144,153,168	0
5	NAG	A	371	14/15	0.38	6.52	82,143,163,164	0
5	NAG	A	331	14/15	0.27	0.78	78,106,119,130	0
5	NAG	C	331	14/15	0.22	0.60	71,92,110,125	0
8	NAG	E	331	14/15	0.20	0.33	68,93,116,121	0
5	NAG	E	351	14/15	0.15	-1.18	108,132,146,146	0
5	NAG	E	352	14/15	0.27	-	115,143,154,156	0
8	NAG	E	332	14/15	0.32	-	100,116,137,142	0
5	NAG	C	332	14/15	0.28	-	100,128,146,150	0
5	NAG	A	332	14/15	0.36	-	87,114,129,133	0
5	NAG	C	342	14/15	0.59	-	113,162,168,172	0
5	NAG	A	372	14/15	0.55	-	136,162,181,182	0
8	BMA	E	333	11/12	0.33	-	89,122,134,135	0

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
7	NAG	C	351	14/15	0.40	13.83	120,155,173,173	0
7	NAG	C	371	14/15	0.44	8.70	83,131,148,149	0
7	NAG	A	341	14/15	0.52	8.12	120,133,141,144	0
9	SO4	E	346	5/5	0.35	5.35	102,122,137,161	0
7	NAG	E	371	14/15	0.39	4.98	91,124,140,144	0
9	SO4	E	340	5/5	0.26	4.74	118,135,172,174	0
9	SO4	L	213	5/5	0.39	4.65	118,126,151,151	0
9	SO4	C	339	5/5	0.40	4.13	118,178,179,184	0
9	SO4	E	345	5/5	0.43	3.85	122,123,146,154	0
9	SO4	E	342	5/5	0.34	3.47	128,128,162,175	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
9	SO4	C	337	5/5	0.34	3.38	114,131,160,169	0
7	NAG	E	341	14/15	0.45	3.35	113,129,137,139	0
9	SO4	I	229	5/5	0.32	3.10	106,113,139,152	0
9	SO4	E	335	5/5	0.29	3.09	106,110,129,145	0
9	SO4	E	339	5/5	0.40	2.73	116,119,140,143	0
9	SO4	A	337	5/5	0.45	2.71	106,115,143,149	0
9	SO4	C	340	5/5	0.34	2.24	106,121,139,155	0
9	SO4	C	338	5/5	0.32	1.87	109,117,134,150	0
9	SO4	I	230	5/5	0.28	1.87	124,151,160,166	0
9	SO4	H	230	5/5	0.31	1.76	126,130,147,157	0
7	NAG	C	361	14/15	0.34	1.52	116,147,153,158	0
9	SO4	H	229	5/5	0.31	1.50	96,110,138,149	0
9	SO4	A	338	5/5	0.20	1.48	113,121,146,148	0
9	SO4	N	213	5/5	0.28	1.44	114,121,137,145	0
7	NAG	E	361	14/15	0.24	1.36	111,128,141,143	0
9	SO4	N	214	5/5	0.23	1.32	122,124,156,171	0
9	SO4	C	336	5/5	0.29	1.21	100,112,135,145	0
9	SO4	C	343	5/5	0.25	1.07	117,121,150,159	0
7	NAG	A	361	14/15	0.36	0.94	116,142,148,148	0
9	SO4	M	212	5/5	0.28	0.73	117,120,132,144	0
9	SO4	N	212	5/5	0.30	0.69	115,125,146,164	0
9	SO4	I	228	5/5	0.24	0.62	84,112,118,141	0
9	SO4	E	336	5/5	0.20	0.46	68,82,98,102	0
9	SO4	J	229	5/5	0.25	0.39	92,110,126,145	0
9	SO4	I	231	5/5	0.17	0.19	64,82,90,92	0
9	SO4	I	232	5/5	0.18	0.14	95,119,139,139	0
9	SO4	L	212	5/5	0.17	0.07	105,113,134,149	0
9	SO4	C	334	5/5	0.18	-0.11	73,76,97,106	0
9	SO4	E	343	5/5	0.17	-0.14	124,134,162,163	0
9	SO4	A	335	5/5	0.16	-0.62	55,88,102,103	0
9	SO4	E	344	5/5	0.15	-0.78	111,113,129,135	0
9	SO4	A	339	5/5	0.25	-0.93	123,125,138,158	0
9	SO4	E	337	5/5	0.21	-1.17	102,102,121,141	0
9	SO4	H	228	5/5	0.11	-1.33	73,78,88,102	0
9	SO4	C	333	5/5	0.15	-1.40	79,87,105,109	0
9	SO4	J	228	5/5	0.10	-1.44	67,74,78,113	0
9	SO4	A	334	5/5	0.11	-2.73	93,95,122,127	0
9	SO4	E	334	5/5	0.11	-3.08	95,98,112,118	0
9	SO4	A	336	5/5	0.14	-3.75	115,130,154,164	0
9	SO4	E	338	5/5	0.12	-8.01	113,116,144,149	0
9	SO4	C	335	5/5	0.13	-13.57	113,119,122,139	0
6	MAN	A	333	11/12	0.33	-	110,121,146,150	0

6.5 Other polymers ⓘ

There are no such residues in this entry.